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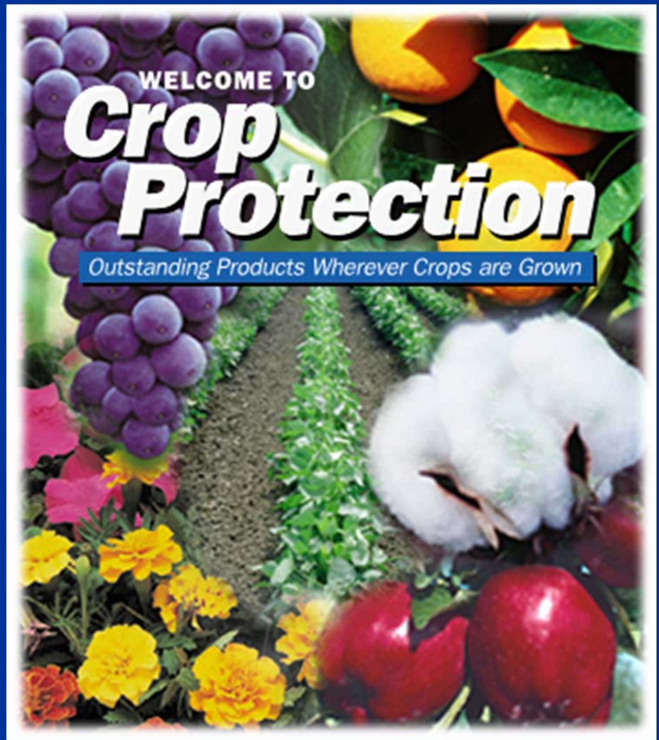

CPD-3285

Jeroen Coppelmans
Igor van der Hel
Vincent Lukkien
Roel Meulendijks

Final Review Meeting
CPD Group 3285
04-02-2003

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Introduction

Crompton

CROMPTON EUROPE BV

- Amsterdam facility
- Producing 2,6-DBN & Diflubam
- Formulation of Casoron 700 ton/a

QUESTION:

“Make a conceptual process design for the production of new ammoxidation products 2-CBN, 4-CBN and/or 3,4-DBN in the existing DBN plant of Crompton Europe B.V. in Amsterdam”

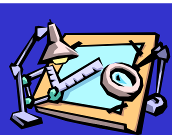
Introduction

Contents

CPD-3285

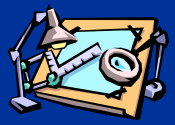
REPORT:

Design of a plant capable of producing 2,6-DBN, 3,4-DBN, 2,6-DFBN and benzonitrile.



Contents

Creativity, Group Process & Tools



Process Design

Design Evaluation

Conclusion

Discussion

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Creativity

Crompton

Group Processes

CREA-TIVITY

Sustainability from Expert

Walk along the Schie

De Bono Hats For Equipment

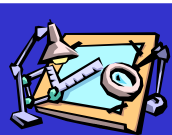
Block Scheme Drawing

Attitude & Creativity

Closing the Eyes

Use of Small Notebook







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Group Process

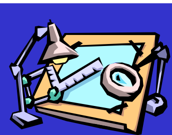
Crompton

Tools

GROUP PROCESS

- Early indication Strengths & Weaknesses and Expectations of group members
  - 3 intermediate evaluation sessions
- Team learning (McKinsey)
  - Bowling / CPD party
- Taking turns in team captain and secretary
  - Have girls over for lunch
  - La Residence

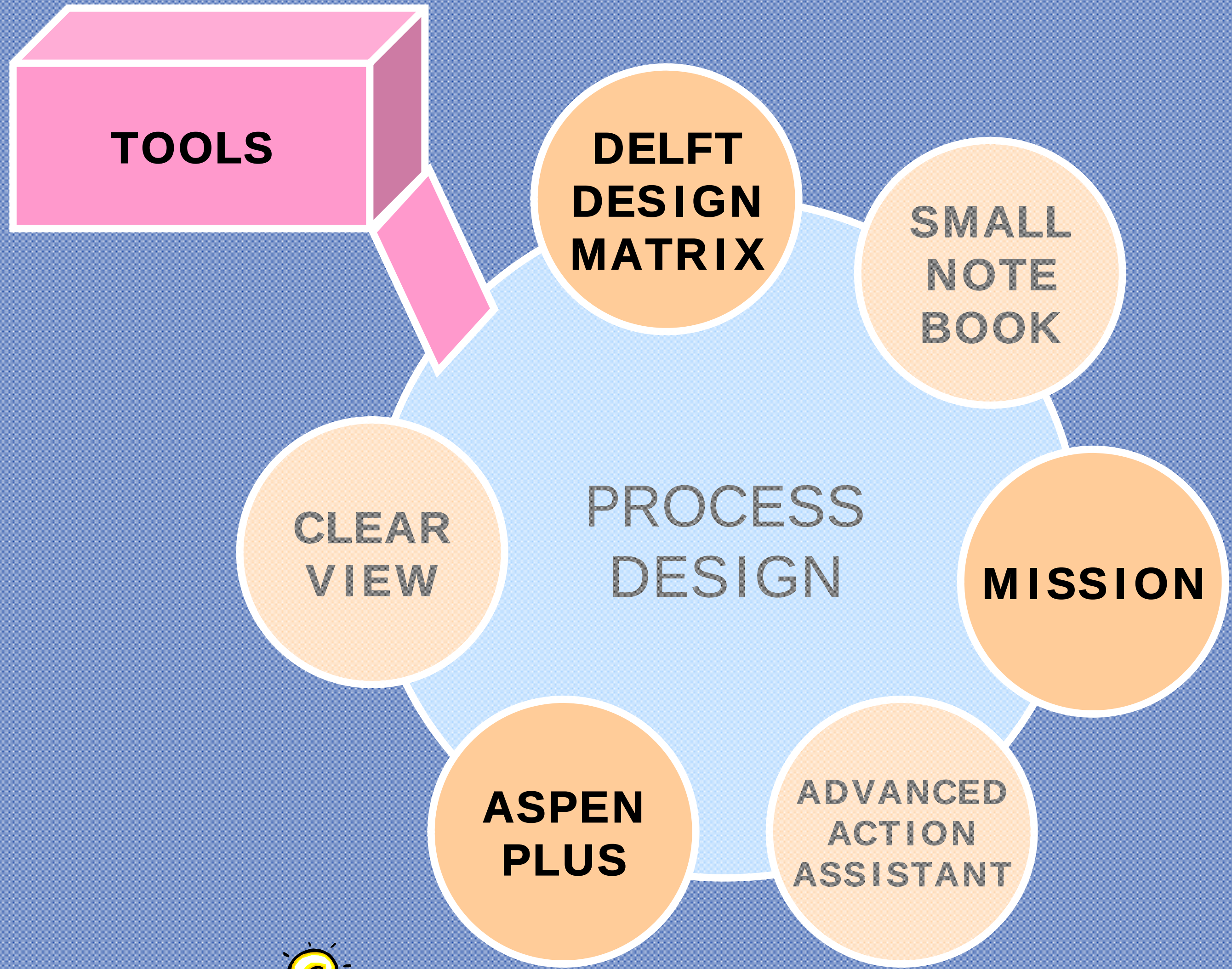




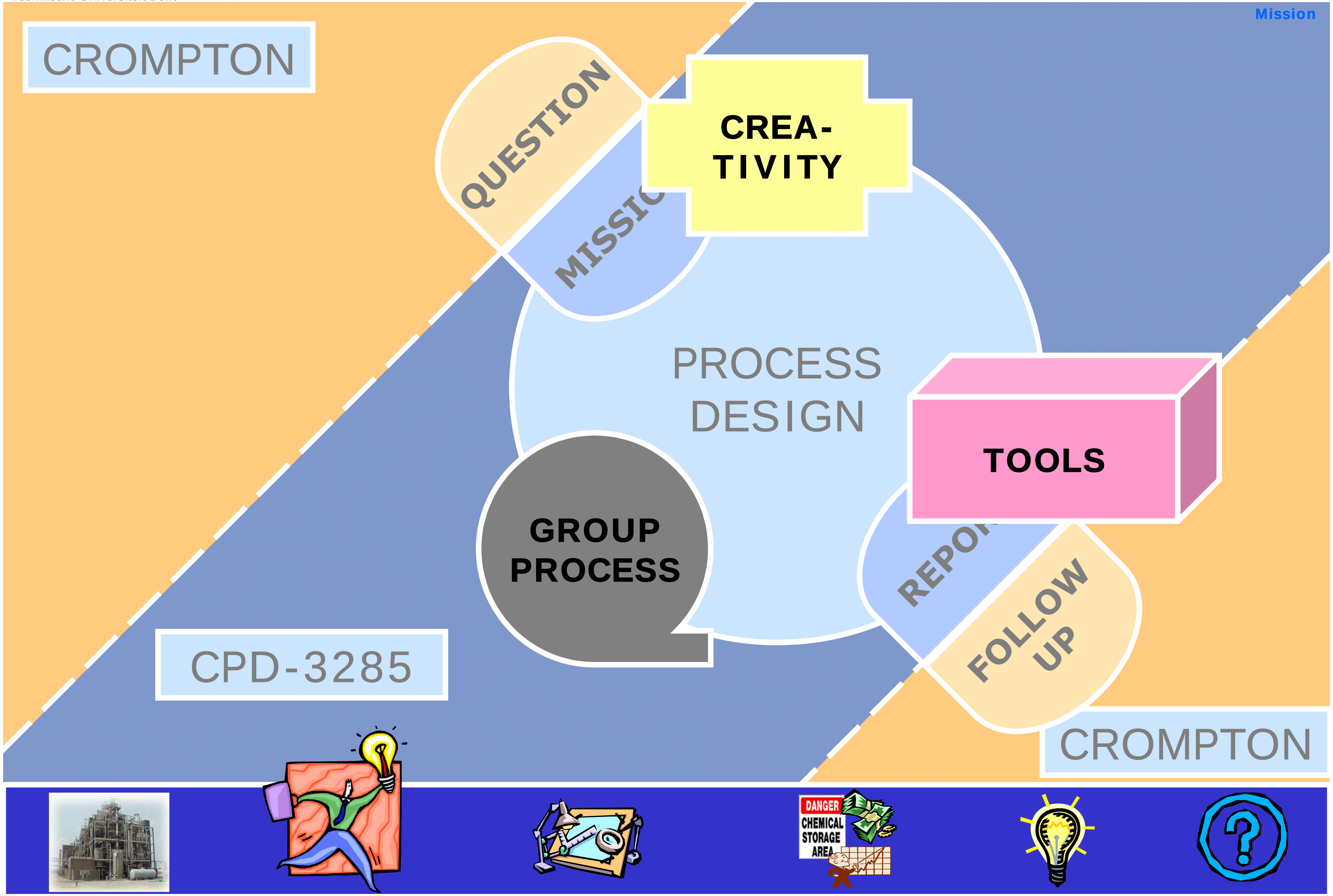


Tools

Mission statement



Mission Statement



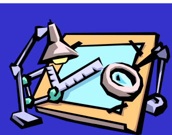
Mission

CPD-3285

MISSION:

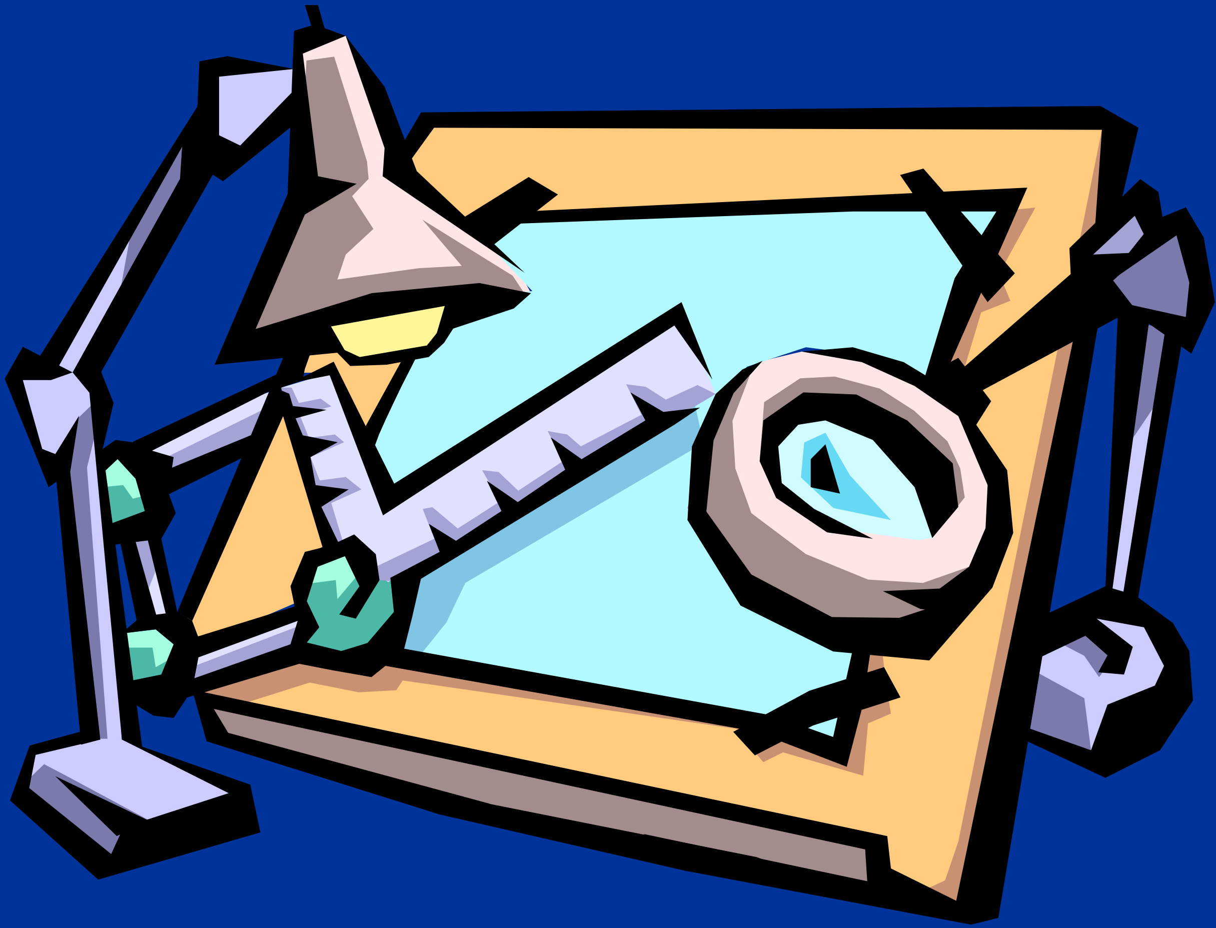
“Design an innovative, sustainable and economic profitable process, which is flexible in the isolation section, for the production of chlorobenzonitriles using present equipment as a basis”







Process Design



Next slide title

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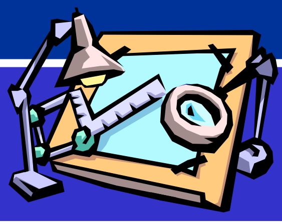
Key Decision Factors

Crompton
Focus of Design

- Technical
  - Use current equipment
  - Flexible isolation section
- Economically Profitable
- Sustainable
- Innovative







Focus of Design

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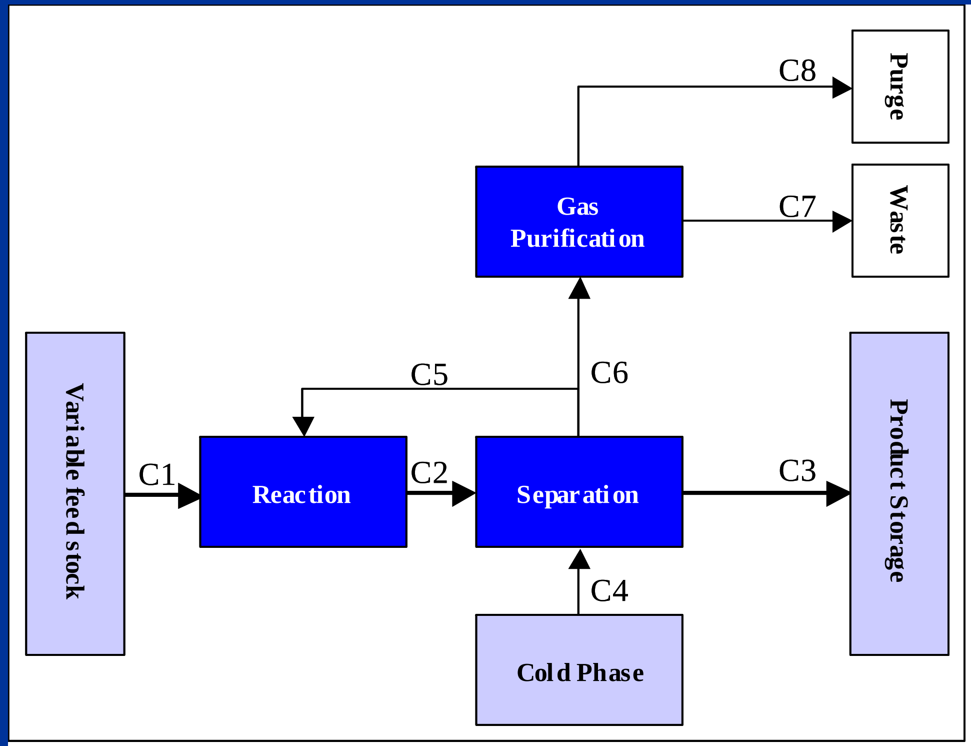
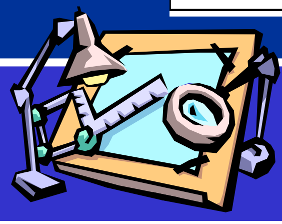
Crompton

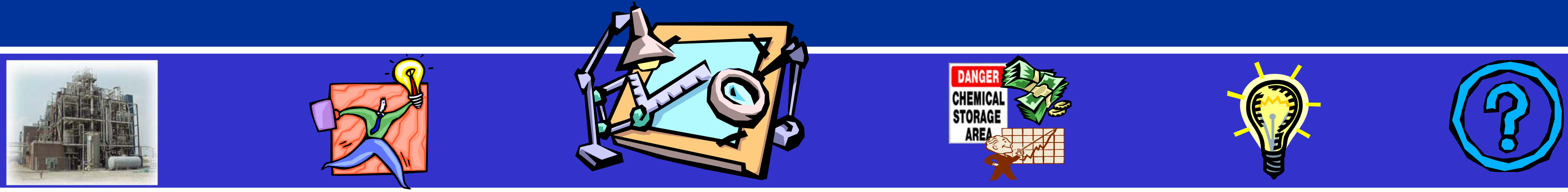
Product Choice

- Product choice
- Operation mode
- Quench





Product Choice



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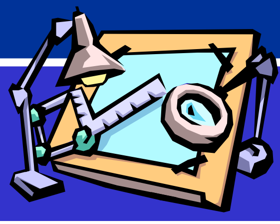
Current situation

- 10 % Crompton revenue is Herbicides
- Amsterdam 2,6 DBN, Diflubam
- Casoron G 700 ton
- Certificates vs Intermediates, lower the cost for production of 2,6 DBN
- Overcapacity



Product choice

Operation mode

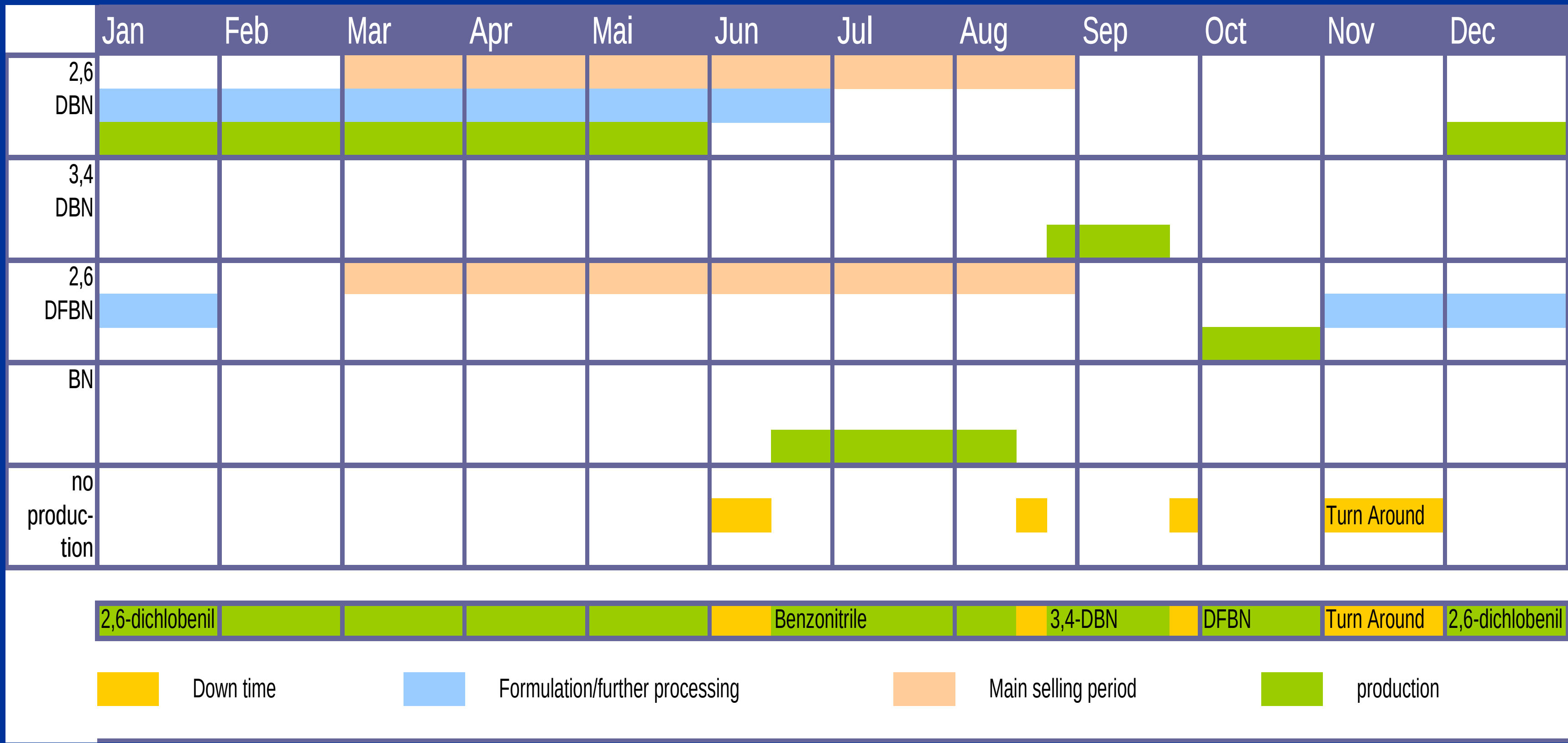
	Economical Profitability	Sustainable	Innovative
2,6-DBN	+	0	N/A
3,4-DBN	+	0	N/A
2,6-DFBN	+	+	N/A
BN	N/A	+	N/A

- Price estimation
- Operability
- Wastes
- Impact on Environment
- No Marketing




Operation Mode

Operation mode results



Operation Mode Results

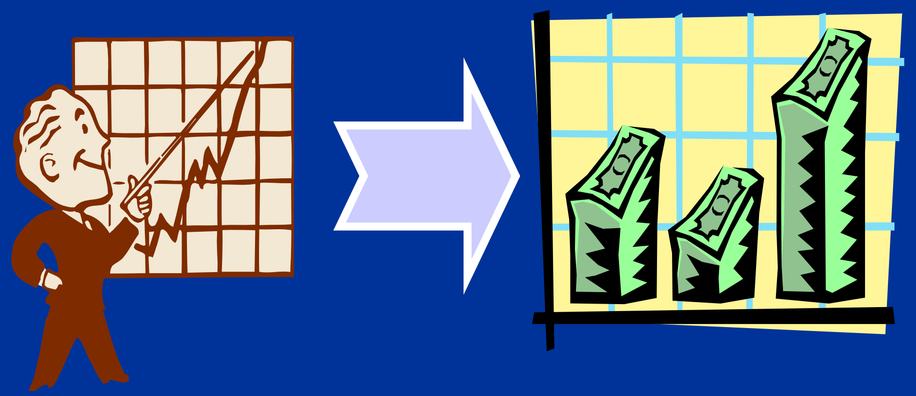
Operation modes

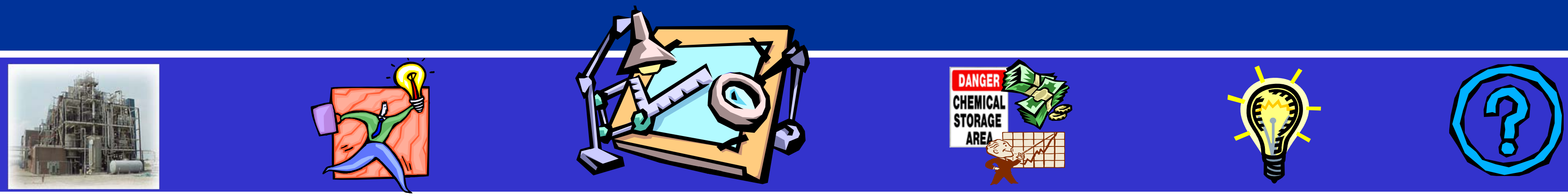
- Series
- Parallel
- Simultaneously

Product choices

- One kind of halogen (Chloro only)
- More Halogens

Produce multihalogens in series on instant market demand





Quench

Quench Approach

Current Process

- Quenching product stream with large amounts of water
- Small particles cause problems in rest process, difficult to separate from slurry phase
- New products with low T_m cannot be crystallized

Solution

- Rigorous change in isolation section

New Process

- Use quench medium that separates from product phase in column
- Quench product to liquid in stead of solid state




Quench medium

- Water
- Ammonia / Oxygen
- Compressed Air
- Solid CO_2
- Liquid Nitrogen
  - + Quench medium leaves at different exit than product stream
  - + Sufficient cooling capacity for relatively low amounts
  - + Inert to reaction, safe (already present in high amounts)
  - + Low temperatures can be reached
  - – Per kg of product 13 kg Nitrogen needed
  - – Fairly expensive





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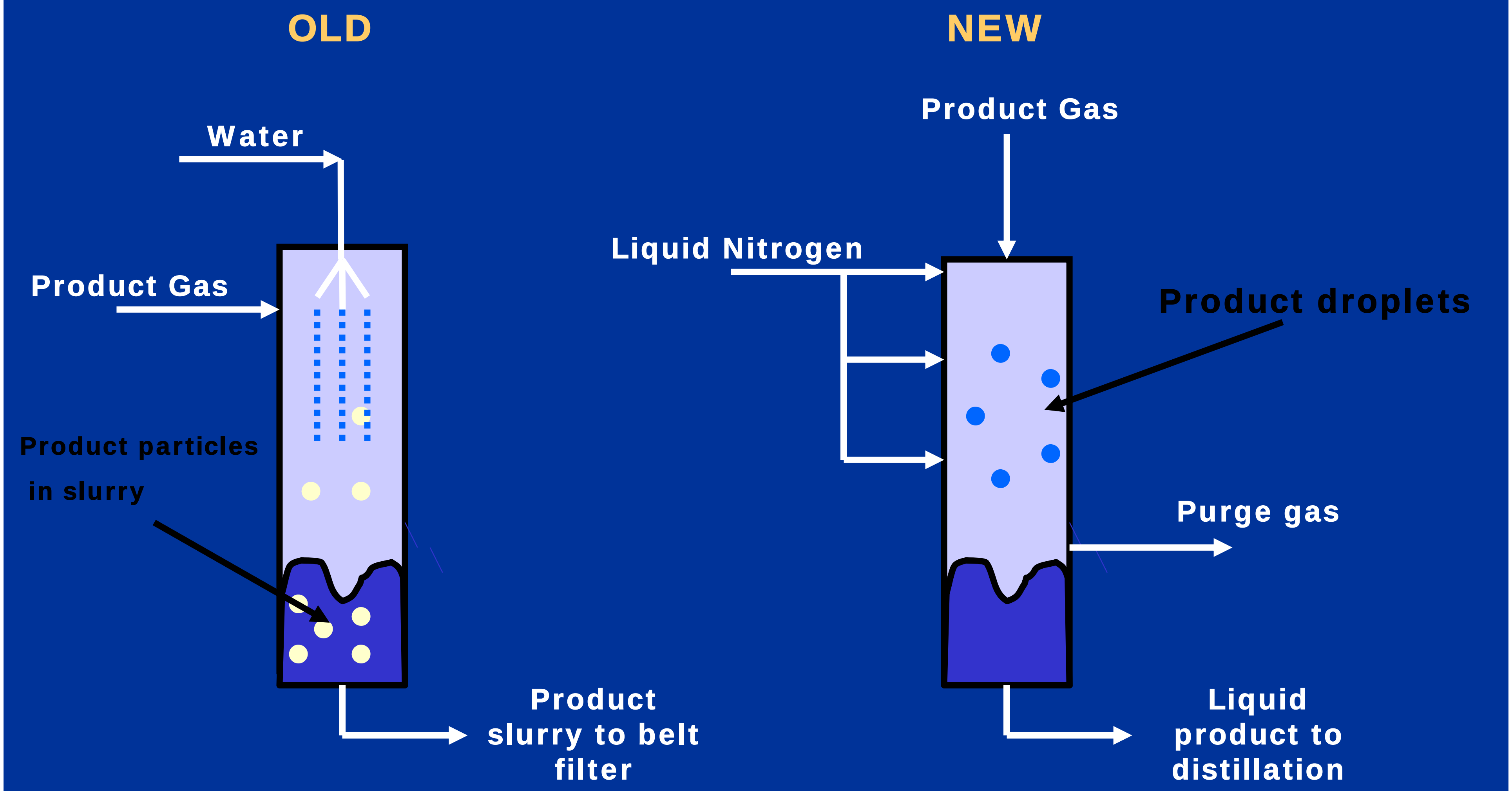
Old vs New Quench

Crompton



Conclusion Quench

- Technical feasible
  - + No heat transfer limitations according to experts (API)
  - + Capable of quenching to low temperature (new products?)
  - + Easy further purification by distillation liquid phase
  - - Transport 2,6-DBN is problem
  - - No examples in industrial practice found
- Economically Profitable
  - - Nitrogen is relatively expensive quenching medium
- Sustainable
  - + Less equipment
  - - Big gas purge
- Innovative
  - + Very original idea by focusing at fundamental problem

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Design Description

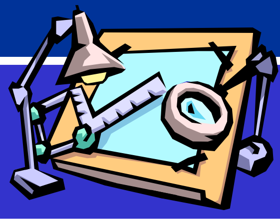
Crompton

A **multipurpose** ammoxidation plant, for the production of:

- 2,6-dichlorobenzonitrile,
- 3,4-dichlorobenzonitrile,
- 2,6-difluorbenzonitrile and
- benzonitrile

from the corresponding (halogen)toluenes **in series** over the **current catalyst**. Instant product choice will be **market driven**. All products are quenched with **liquid nitrogen**. The products are **liquids** at quench temperature and are isolated in a **distillation process**. The current plant remains intact.







Process Flow Scheme

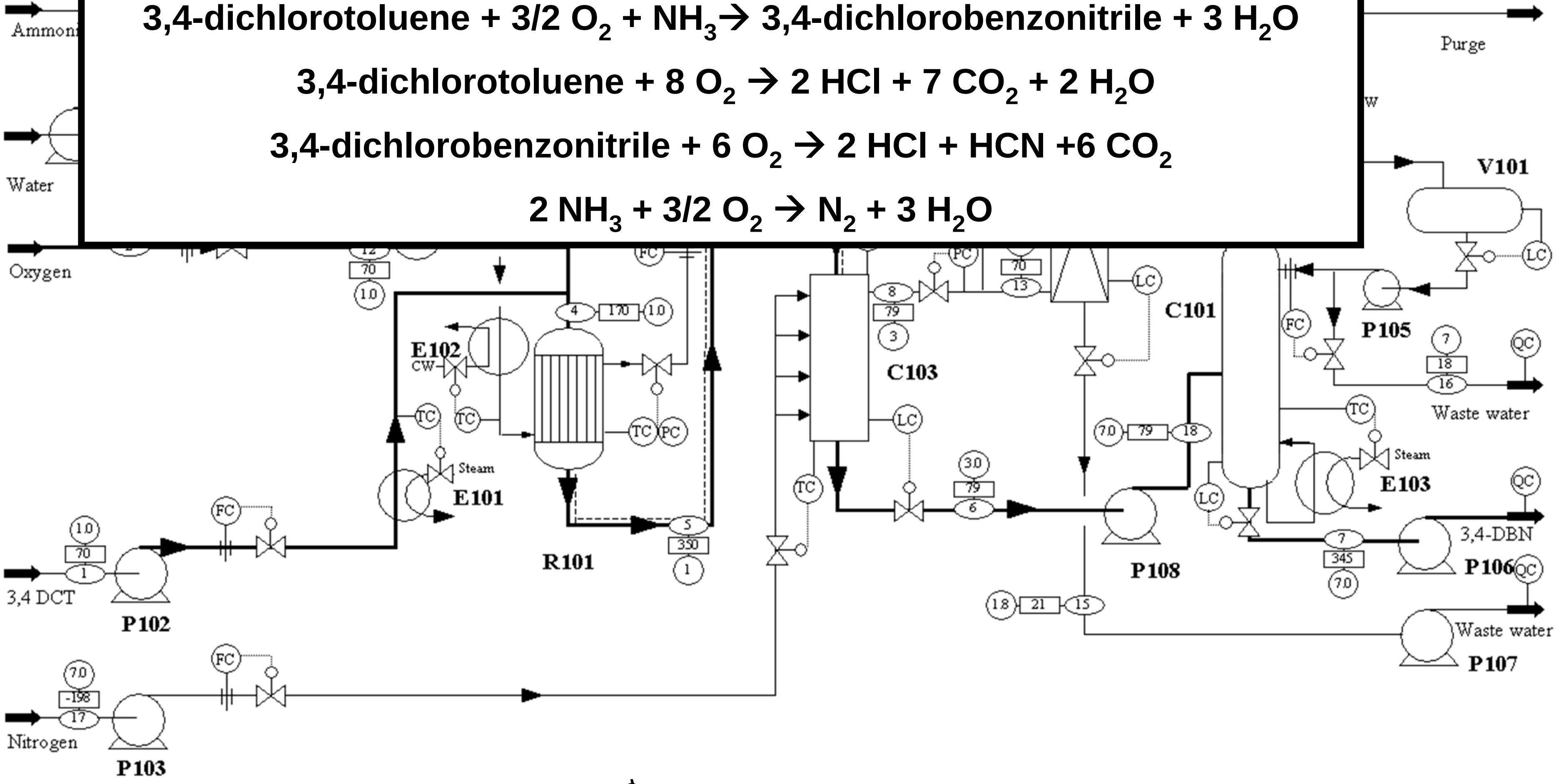
Reactions

$$\text{3,4-dichlorotoluene} + 3/2\ O_2 + NH_3 \rightarrow \text{3,4-dichlorobenzonitrile} + 3\ H_2O$$

$$\text{3,4-dichlorotoluene} + 8\ O_2 \rightarrow 2\ HCl + 7\ CO_2 + 2\ H_2O$$

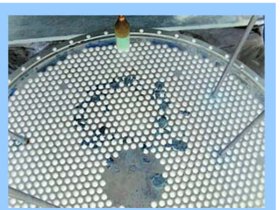
$$\text{3,4-dichlorobenzonitrile} + 6\ O_2 \rightarrow 2\ HCl + HCN + 6\ CO_2$$

$$2\ NH_3 + 3/2\ O_2 \rightarrow N_2 + 3\ H_2O$$



Equipment design

Reactor



- Current reactor
- P = 1 bar
- T = 330-370^{o}C

Gas absorber

- Problem: no convergence above 8 trays
- 4500 kmol/hr is too much water
- 13 trays will be better
- New column needed, due to higher gas duty

Quench

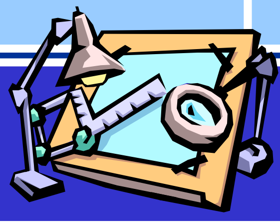
- Optimize bottom product stream
- P >, T<, keeping product liquid
- 2,6 DBN liquid slurry
- Use current quench column,
    - Vs = 2.3 tau = 5s
- P = 1-4.5 bar
- Hot streams enter in top, cold leave bottom

Distillation Column

- Water amount bottom 0.5 %
- T top > 15^{o}C
- 6 trays
- P = 1-20 bar
- Reflux 1.2
- Yield over 99.5 %

Other Design Issues







Other Design Issues

- **HF is no problem in diluted gas stream**

  Concentrations V = 0.004 %w

  L = 0.00078 %w

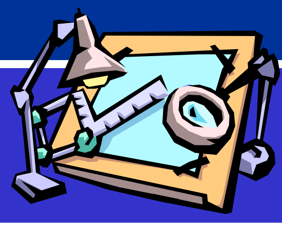
  =>0.25 mm corrosion/year

  – **increase tube wall thickness**

- **Changes outside battery limit**
  - **Crystallizer: cold roller**
  - **Raw material storage**
  - **Waste water treatment**

- **Current plant remains intact**







Design Evaluation

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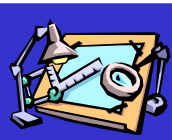
Process Safety

Wastes

- HAZOP over Quench
  - Maintaining temp in Quench is important
- Fire and Explosion Index (FEI) over all units
  - Overall process is light to somewhat moderate hazardous
  - Look out for leakages, HF, HCl and HCN are present!!!
  - Process is not risk-free



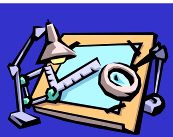




Wastes

- Less waste by eliminating 2,6-DFBN process in other plant
- Waste water
  - (problems with absorber, therefore high volume)
- HCl is key component in gas purge treatment
- HF purge does not come close to environmental limits
- Not fair to compare a real plant to a conceptual model







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Economics

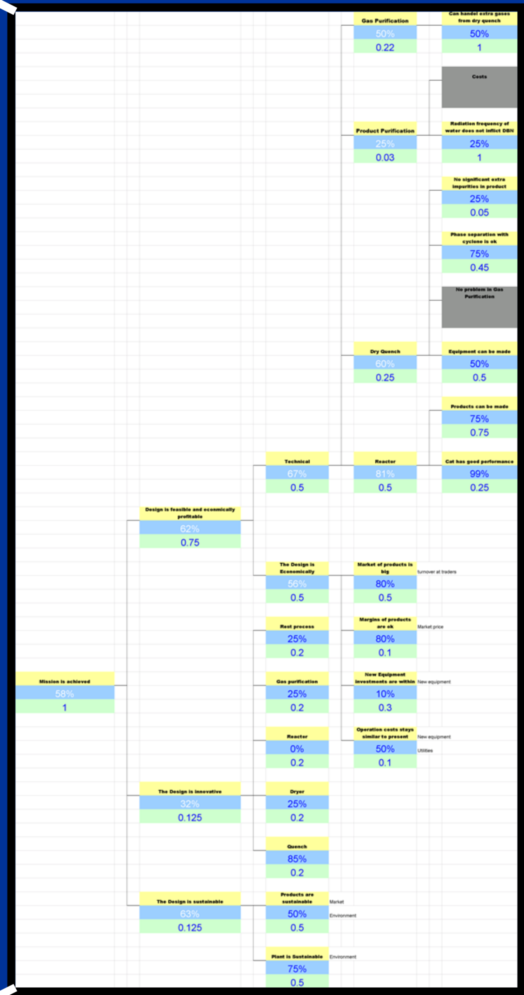
Crompton

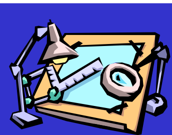
Uncertainty tree

- Production of Benzonitrile is not economically profitable
- Producing 2,6-DFBN and 3,4-DBN for 5 months
  - Total investments: M$ 1.8
  - Total operational costs: M$ 14.3 / year
  - Cash flow: M$ 0.5 / year
  - DCFROR: 20.0 %
- Major uncertainty: prices raw materials and products
- New plant lowers cost price of 2,6-DBN with $ 0.75 per kg

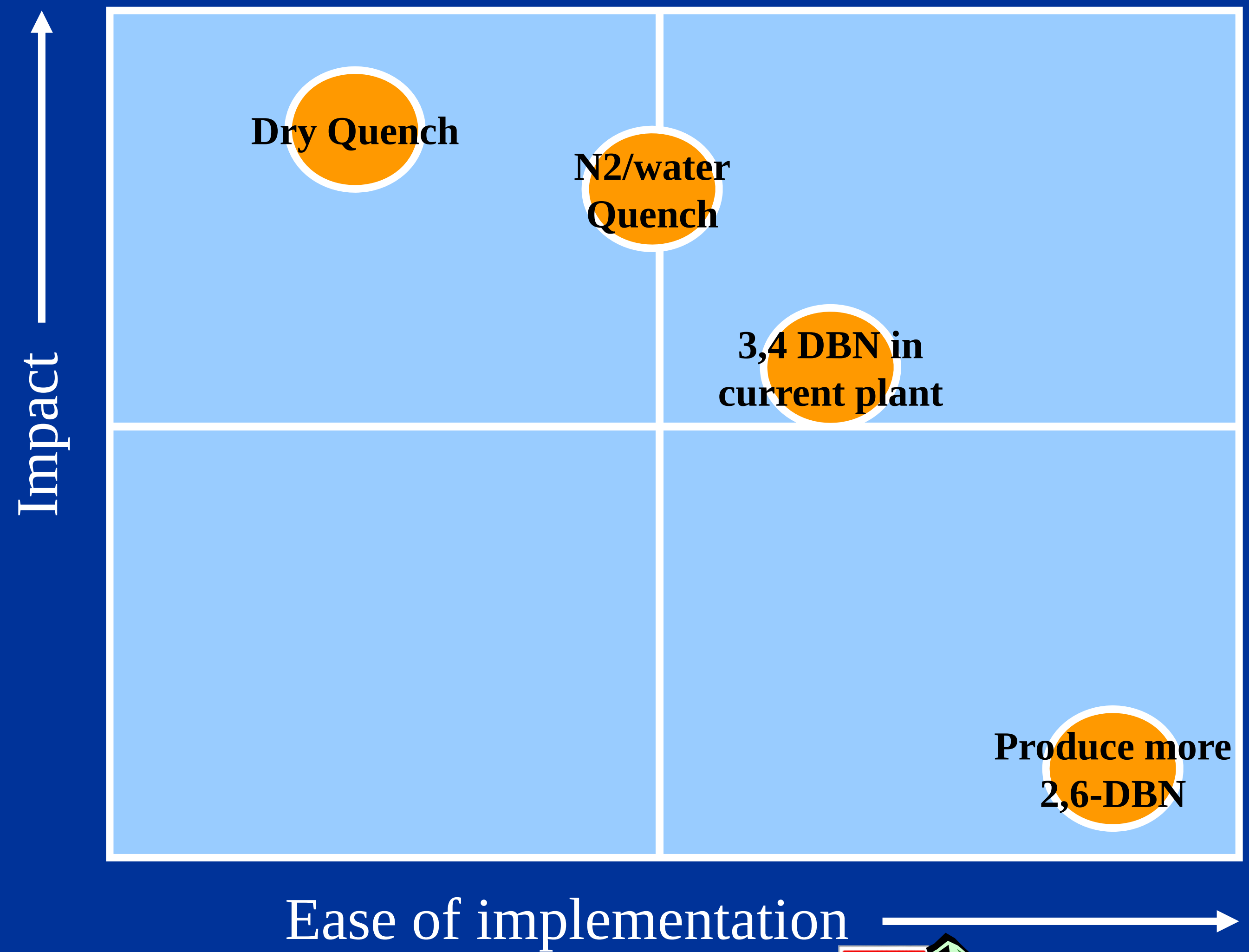
Uncertainty Tree

Valuable Improvements





Valuable improvements



Conclusions

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Decision Keys

Crompton

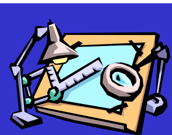
Technical Feasibility

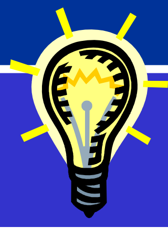
+ A multipurpose plant is designed for the production of
  - 3,4-DBN,
  - 2,6-DFBN and
  - Benzonitrile
- Production of 2,6-DBN is most probably technically infeasible in the designed plant
+ Reactor and quench column can also be used for other ammoxidation processes

Economical profitability

+ $0.75 per kg cost reduction on 2,6-DBN after investments are paid back
- Production of Benzonitrile is economically not profitable






Decision Keys

Sustainability

- \+ Make 2,6-DFBN, so the unsustainable diflubam process can be omitted.
- \+ A flexible plant is sustainable, because it will not become obsolete if market demands for its product decreases. New products can then be made.
- \+ A higher mass based yield is obtained for 3,4-DBN than for the current 2,6-DBN process
- \- Large waste water stream for 3,4-DBN and 2,6-DBN.
- \- Large amount of Nitrogen needed for quench

Innovativity

- \+ Dry Quench. Reduces difficulties in purification section considerably

Recommendations

Crompton Valuables

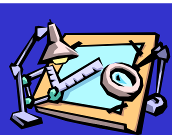
- Produce 2,6-DBN in current process
- Short time perspective
  - Produce 3,4-DBN in current process
- Long term perspective
  - Develop dry quench further for production of 2,6-DFBN and 3,4-DBN

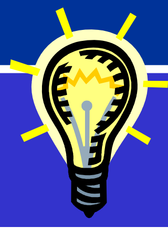
Crompton valuables

CPD

- Market research results
- Catalyst research results
- Chemical properties possible products
- Dry Quench idea
- Diflubam production in new plant
- Aspen models for all products
- Loose end list
- Literature file





Creativity
Produces
Dreams

Discussion

Subject Inventory

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- …
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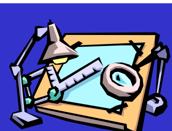

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Technical details

Crompton

Next slide title

Technical details

- Contents
  - Quench Calculations
  - Price estimation
  - NRTL model Selection
  - Mass and Heat balances
  - Thermodynamics calculations
  - Physical properties chemicals used
  - Current process block scheme
  - Aspen model
  - HF in equipment

Quench Calculations

Required cooling in Quench column

All calculations are made for the case of 2,6-DBN

Temperature reactor out: 330 degrees celcius

Temperature quench out: 70 degrees celcius

Cooling all components from Treactor out to Tquench out:

	Mass stream	*Cp*	*Molar mass*	*Cp*	*Delta T*	*Q*	*Q*	*% of total*
	kg/hr	*J/(mol K)*	*g/mol*	*J/(kg K)*	*K*	*J/kg*	*J*	
Nitrogen	2276	29	28	1039	260	2.70E+05	6.15E+08	72%
Dichlobenil	172	140	172	814	260	2.12E+05	3.64E+07	4%
H2O	112	35	18	1944	260	5.06E+05	5.66E+07	7%
CO2	41	38	44	864	260	2.25E+05	9.21E+06	1%
CO	296	30	37	1037	260	2.70E+05	7.98E+07	9%
NH3	60	37	17	2176	260	5.66E+05	3.40E+07	4%
Total	2957						8.31E+08	97%

Desublimizing dichlobenil

	Mass stream	*Hsub*		*Hsub*		
	kg/hr	*J/mol*	*Molar mass*	*J/kg*		
Dichlobenil	172	2.62E+04	172	1.52E+05	2.62E+07	3%
				Total heat to be removed in 1 hour	**8.57E+08**	100%

Quench Calculations

Cooling with nitrogen

Pin:	200 bar	*Tin:*	20 degr. C	*gas*
Pout:	1 bar	*Tout:*	70 degr. C	*gas*

	Avg. MM	*p1*	*p2*	*Q=Rtlin(p1/p2)*	*Q*
	g/mol	*pa*	*pa*	*J/mol*	*J/kg*
Pin-->Puit	28.00	2.00E+07	1.00E+05	1.29E+04	4.61E+05

	Cp	*Delta T*		*Q*
	J/(kg K)	*K*		*J/kg*
Tin-->Tuit	1.04E+03	50		5.20E+04
			Total	5.13E+05

Required cooling capacity (see Appendix 1): 8.57E+08 J/hr

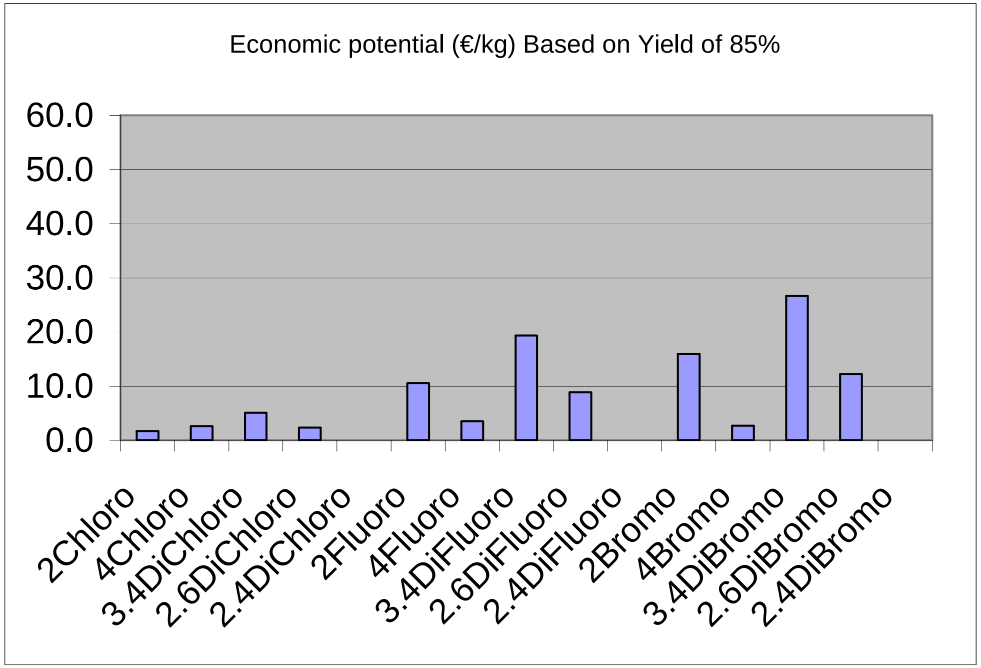
Needed massflow of compressed air: 1670 kg/hr

This would result in the following volume flows:

rho gas at p1	*Volumeflow at p1*
kg/m3	*m3/hr*
230	7
rho gas at p2	Volumeflow at p2
kg/m3	m3/hr
1.15	1452

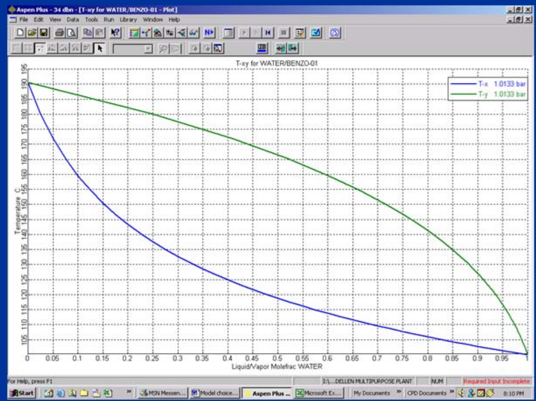
Price estimation

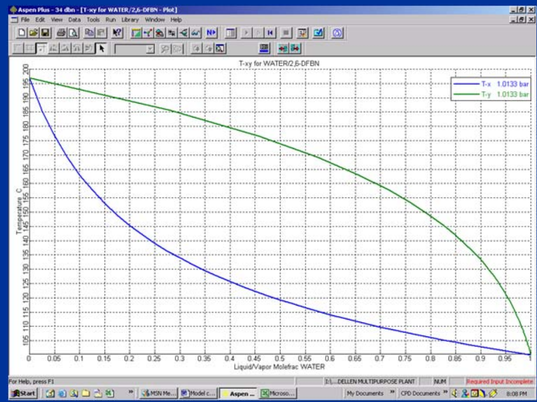
Benzonitrile	Economic potential (€/kg)	Product price (€/kg)	Profits per kg Raw material (€/k	Raw Material cost (€/kg)	Toluene
2Chloro	1.7	**8**	**7**	5	2Chloro
4Chloro	2.6	**12**	**10**	8	4Chloro
3.4DiChloro	5.1	**24**	**20**	15	3.4DiChloro
2.6DiChloro	2.4	**11**	**9**	**7**	2.6DiChloro
2.4DiChloro					2.4DiChloro
2Fluoro	10.6	**35**	**30**	19	2Fluoro
4Fluoro	3.5	**38**	**32**	29	4Fluoro
3.4DiFluoro	19.3	91	77	58	3.4DiFluoro
2.6DiFluoro	8.9	41	35	26	2.6DiFluoro
2.4DiFluoro					2.4DiFluoro
2Bromo	16.0	**50**	**43**	27	2Bromo
4Bromo	2.7	**50**	**43**	40	4Bromo
3.4DiBromo	26.7	125	106	80	3.4DiBromo
2.6DiBromo	12.2	57	49	36	2.6DiBromo
2.4DiBromo					2.4DiBromo

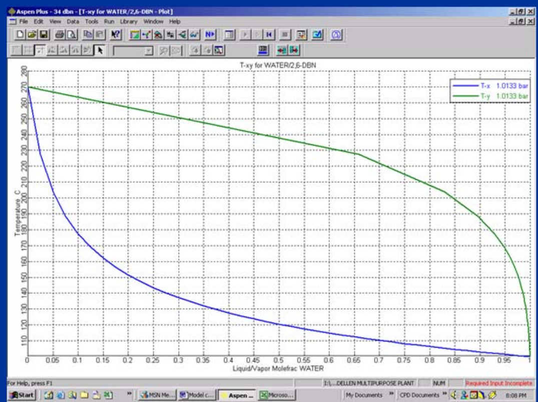


NRTL model Selection

NRTL Water in product







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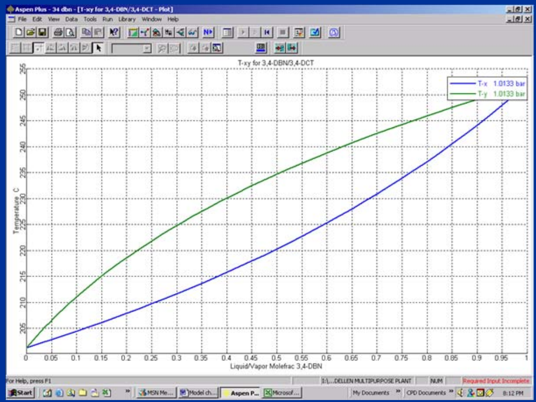
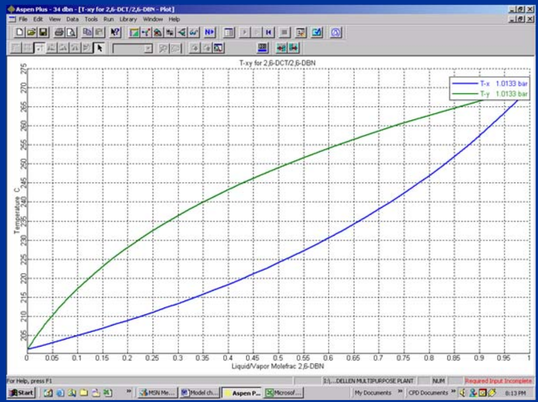
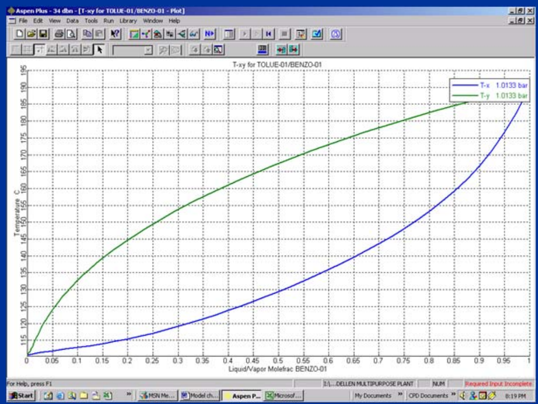
NRTL model Selection

Crompton

NRTL Raw material in product

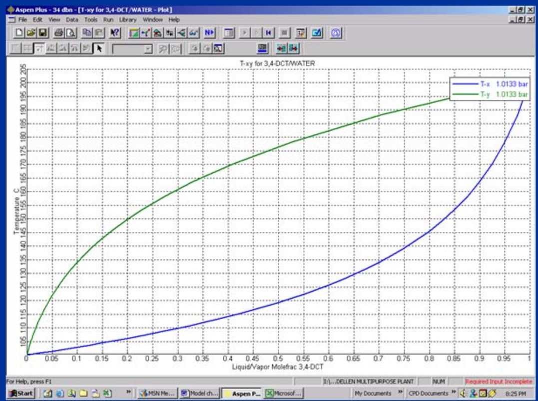


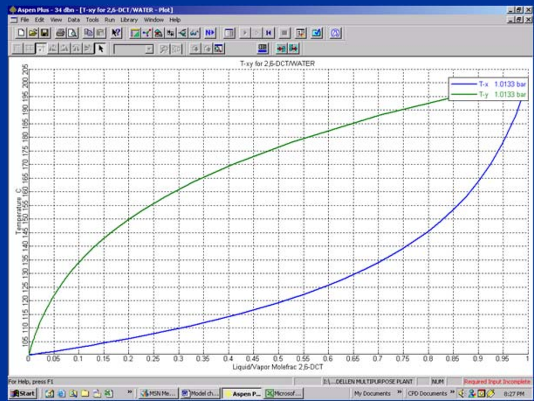


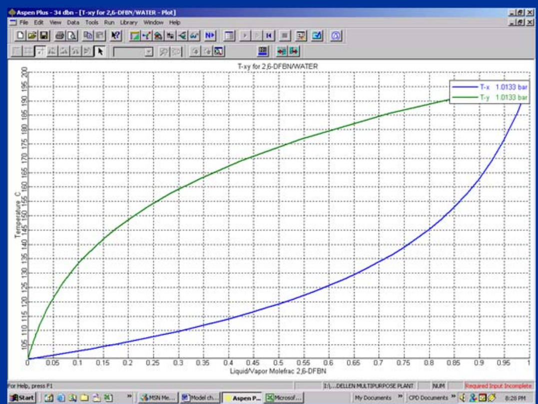


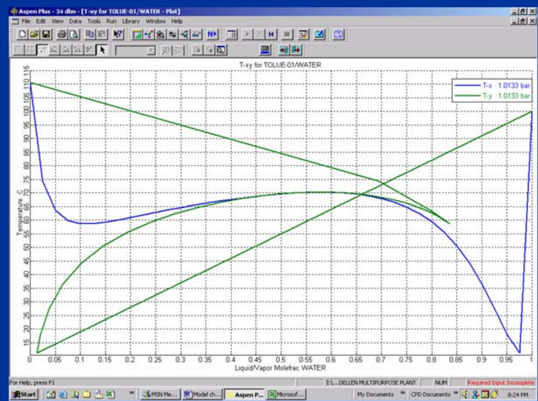
NRTL model Selection

NRTL Water in raw material



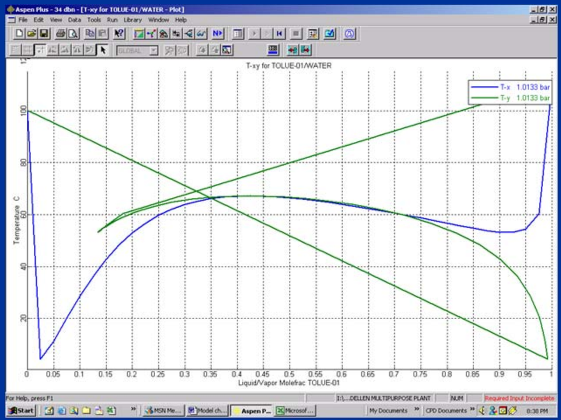




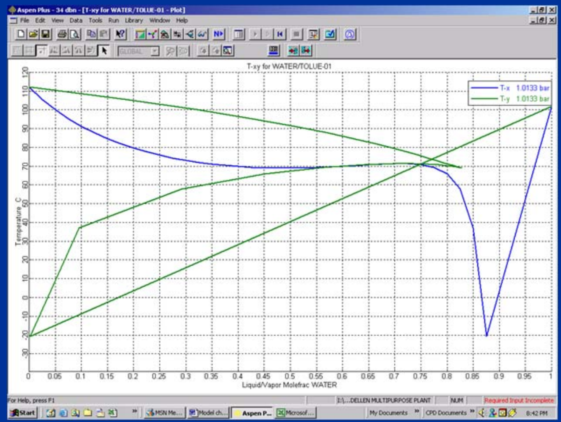


NRTL model Selection

Uniquac: Water in Toluene



Peng Robinson: Water in Toluene



Mass and Heat balances

The reaction process

3,4-dichlorotoluene + 3/2 O_2 + NH_3 → 3,4-dichlorobenzonitrile + 3 H_2O

3,4-dichlorotoluene + 8 O_2 → 2 HCl + 7 CO_2 + 2 H_2O

3,4-dichlorobenzonitrile + 6 O_2 → 2 HCl + HCN +6 CO_2

2 NH_3 + 3/2 O_2 → N_2 + 3 H_2O

Mass balance

$$\phi_{M,A,out} = \sum_{i=1} \upsilon_A \cdot \xi_{A,i} \cdot \phi_{M,A,in}$$

Heat balance

$$Q_{HE} = \left(\phi_{M,x,in} - \phi_{M,x,out}\right) \cdot C_{P,x} \cdot \left(T_{in} - T_{out}\right) - \Delta_r H$$

Mass and Heat balances

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The quench process

Mass balance

$$0 = \phi_{M,Quenchmedium,in} + \phi_{M,Gas,in} - \phi_{M,Liquid,out} - \phi_{M,Gas,out}$$

Heat balance

$$0 = \left(\phi_{M,Quenchmedium} \cdot C_{P,Quenchmedium} \cdot T\right)_{Liquid,in} + \left(\phi_{M,x} \cdot C_{P,x} \cdot T\right)_{Gas,in} - \left(\phi_{M,x} \cdot C_{P,x} \cdot T\right)_{Liquid,out} - \left(\phi_{M,x} \cdot C_{P,x} \cdot T\right)_{Gas,out}$$

Distillation

Mass balance

$$0 = \phi_{M,in} - \phi_{M,Bottom,out} - \phi_{M,Top,out}$$

Heat balance

$$0 = \left(\phi_{M,x} \cdot C_{P,x} \cdot T\right)_{in} - \left(\phi_{M,x} \cdot C_{P,x} \cdot T\right)_{Bottom,out} - \left(\phi_{M,x} \cdot C_{P,x} \cdot T\right)_{Top,out} + \Delta H_{reboiler} - \Delta H_{Condensor}$$

Purification section

Mass balance

$$0 = \phi_{M,Water,in} + \phi_{M,Gas,in} - \phi_{M,Liquid,out} - \phi_{M,Gas,out}$$

Heat balance

$$0 = \left(\phi_{M,water} \cdot C_{P,water} \cdot T\right)_{Liquid,in} + \left(\phi_{M,x} \cdot C_{P,x} \cdot T\right)_{Gas,in} - \left(\phi_{M,x} \cdot C_{P,x} \cdot T\right)_{Liquid,out} - \left(\phi_{M,x} \cdot C_{P,x} \cdot T\right)_{Gas,out}$$

Thermodynamics calculations

UNIFAC Values

	$\Delta_f H^0$	S^0	C_P^0	G^0
	kJ/mole	J/mole·K	J/mole·K	kJ/mole
	1bar, 350°C	1bar, 350°C	1bar, 350°C	1 bar, 350°C
NH_3	-32.65	-69.35	46.02	10.56
O_2	9.98	22.50	32.32	-4.04
CO_2	-379.47	34.28	47.71	-400.83
HCl	-82.80	31.58	29.68	-102.49
HF	-263.86	28.50	29.35	-281.62
HCN	148.30	64.46	44.29	108.13
H_2O	-230.50	-18.79	36.67	-218.79
N_2	9.59	21.71	30.26	-3.93
Toluene	101.21	-130.02	200.90	182.23
Benzonitrile	265.85	-310.00	191.99	285.17

Shomate's Values

	$\Delta_f H^0$	S^0	C_P^0	G^0
	kJ/mole	J/mole·K	J/mole·K	kJ/mole
	1bar, 350°C	1bar, 350°C	1bar, 350°C	1 bar, 350°C
NH_3	-32.66	222.33	45.99	-56.87
O_2	10.07	227.80	32.48	1.57
CO_2	-379.52	245.07	47.87	-404.23
HCl	-82.80	208.47	29.67	-212.67
HF	-263.07	195.27	29.25	-384.73
HCN	148.32	231.35	44.25	4.19
H_2O	-230.49	214.42	36.58	-364.07
N_2	9.64	213.37	30.60	-123.29

Shomate's Equation

$$C_P^0 = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + \frac{E}{T^2}$$

$$H^0 - H^0_{298.15} = A \cdot T + \frac{B \cdot T^2}{2} + \frac{C \cdot T^3}{3} + \frac{D \cdot T^4}{4} - \frac{E}{T} + F - \Delta_f H^\circ_{298}$$

$$S^0 = A \cdot \ln(T) + B \cdot T + \frac{C \cdot T^2}{2} + \frac{D \cdot T^3}{3} - \frac{E}{2 \cdot T^2} + G$$

Values for the constants are given in Appendix 4.1

Thermodynamics calculations

UNIFAC Values

	$\Delta_f H^0$	S^0	C_P^0	G^0
	kJ/mole	J/mole·K	J/mole·K	kJ/mole
	1bar, 298 K	1bar, 298 K	1bar, 298 K	1 bar, 298 K
Toluene	49.8	-245.1	106.8	120.2
3,4-DCT	-14.3	-281.2	143.2	66.3
2,6-DFT	-331.7	-148.3	141.5	-289.7
2,6-DCT	-14.3	-277.6	143.2	210.2
Benzonitrile	215.1	-145.3	112.4	256.5
3,4-DBN	167.9	-784.6	145.9	394.9
2,6-DFBN	-162.9	-28.7	147.3	-155.7
2,6-DCBN	163.6	-156.4	153.4	68.4

Benson's Values

	$\Delta_f H^0$	S^0	C_P^0	G^0
	kJ/mole	J/mole·K	J/mole·K	kJ/mole
	1bar, 25°C	1bar, 25°C	1bar, 25°C	1 bar, 25°C
Toluene	50	-241.9	94.7	122.1
3,4-DCT	-23.4	420.7	126.5	-148.8
2,6-DFT	-367.4	406.9	119.3	-488.7
2,6-DCT	-23.4	420.7	126.5	-148.8
Benzonitrile	218.9	327.1	109.7	121.4
3,4-DBN	168.7	379.2	142.4	55.7
2,6-DFBN	-175.4	365.4	135.3	-284.3
2,6-DCBN	168.7	379.2	142.4	55.7

Thermodynamics calculations

Equations

$$\Delta_{reaction}H^0 = \sum_i \upsilon_i \cdot \Delta_f H^0$$

$$\Delta_{reaction}G^0 = \sum_i \upsilon_i \cdot G^0$$

$$\Delta_{reaction}G^0 = -RT\ln\left(K\right)$$

dH, dG of reaction and Chemical Equilibrium Constant

Reaction		$\Delta_{reaction}H^0$	$\Delta_{reaction}G^0$	K
		1 bar, 350°C [kJ/mole]	1 bar, 350°C [kJ/mole]	1 bar, 350°C
1	Ammoxidation of 3,4-DCT	-558.74	-164.72	∞
2	Oxidation of 3,4-DCT	-3410.6	-3551.6	∞
3	Oxidation of 3,4 DCBN	-2582.25	-3133.6	∞
1	Ammoxidation of 2,6-DFT	-570.75	-572.96	∞
2	Oxidation of 2,6-DFT	-3455.79	-3509.5	∞
3	Oxidation of 2,6-DFBN	-2615.43	-2665	∞
1	Ammoxidation of Toluene	-574.748	-557.93	∞
2	Oxidation of Toluene	-3769.32	-3826.8	∞
3	Oxidation of Benzonitrile	-2924.96	-2991.3	∞
4	Oxidation of NH_3	-762.18	-675.36	∞

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Physical properties chemicals used

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*PURE COMPONENT PROPERTIES *1)*									
Component name		Technological Data					Medical Data		Note
Design	Systematic	Formula	Mol weight	Boiling point	Melting point	Liq./Sol. Density [6]	MAC value [2]	LD50	
				°C	°C	kg/m3	ppm	ppm	
Oxygen	Oxygen	O_2	32	-182.9	-218.8	1141	n.a.	n.r.	
Ammonia	Ammonia	NH_3	17	-33	-77.7	700	*25*	*7338*	[1] [3]
Water	Dihydrogenoxide	H_2O	18	100	0	997	d.n.e.	n.r.	
2,6-DBN	2,6-Dichlorobenzonitril	$C_7H_3NCl_2$	172	270	144	n.a.	n.a.	*2710*	[4]
2,6-DCT	2,6-Dichlorotoluene	$C_7H_6Cl_2$	161	196	2	1254	n.a.	n.a.	[5]
3,4-DBN	3,4-Dichlorobenzonitril	$C_7H_3NCl_2$	172	252	69	n.a.	n.a.	1600	[4]
3,4-DCT	3,4-Dichlorotoluene	$C_7H_6Cl_2$	161	200	-15.2	1251	n.a.	n.a.	[5]
2,6-DFBN	2,6-Difluorobenzonitril	$C_7H_3NF_2$	139	197	29	n.a.	n.a.	n.a.	
2,6-DFT	2,6-Difluorotoluene	$C_7H_6F_2$	128	112	n.a.	1129	n.a.	n.a.	
Toluene	Toluene	C_7H_8	92	110	-95	865	n.a.	636	[4]
Benzonitrile	Benzonitrile	C_7H_5N	103	190	-13	*1020*	n.a.	971	[4]
CO2	Carbondioxide	CO_2	44	d.n.e.	*-78.5*	1524	5000	n.a.	[8] [10] [13]
HCl	Hydrochloric acid, anh.	HCl	36.5	110	-25	n.a.	5	900	[8] [11]
HF	Hydrofluoric acid, anh.	HF	20	20	-83	997	3	n.a.	[8]
HBr	Hydrobromo acid, anh.	HBr	81	-66.7	-87	2200	3	*2860*	[8] [3]
HCN	Cyanide acid	HCN	27	25.6	-14	690	10	3.7	[8] [12]
N2	Nitrogen	N_2	28	-195.8	-209.9	n.a.	n.r.	n.r.	
30w% HCl (aq)	Hydrochloric acid, hydr.	HCl (aq)	n.r.	110	0	1200	5	900	[11]
49w%HF (aq)	Hydrofluoric acid, hydr.	HF(aq)	n.r.	103-10	-35	1150	3	342	[13]

***1)** Data from MSDS/ICSC unless mentioned
[1] TLV i.s.o. MAC
[2] ppm
[3] LC50 (ppm) i.s.o. LD50
[4] oral **rat** mg/kg
[5] solid density g/cm3
[6] At 101.3 kPa, 21°C, kg/m3
[7] Data from Handbook of Chemistry and Physics 81st edition
[8] Data from 'Nationale lijst van Mac-waarden, 1985'
[9] LC50 (ppm) mouse i.s.o. LD50
[10] sublimation point
[11] oral rabbit mg/kg
[12] oral mouse mg/kg
[13] b.p. CO_2 d.n.e. at normal pressure (solid→vapour tranfer)

n.a. = not available
d.n.e. = does not exist (physically)
n.r. = not relevant

Physical properties chemicals used

PURE COMPONENT PROPERTIES (cont.)									
Component name		Technological Data					Safety data		Note
Design	Cas number	Vapour pressure [1]	Auto Ignition T	Flash point	Tcritic	Vapour Density [1]	LEL	UEL	
		mmHg	°C	°C	°C	kg/m3	%	%	
Oxygen	7782-44-7	d.n.e.	d.n.e.	d.n.e.	-118.4	1.326	d.n.e.	d.n.e.	**[2]**
Ammonia	231-635-3	.	630		132	0.717	15	30	**[2]**, [3]
Water	7732-18-5	17.5	d.n.e.	d.n.e.			d.n.e.	d.n.e.	
2,6-DBN	1194-65-6		527	216					**[2]**
2,6-DCT	118-69-4			79/82		5.6			**[2]**
3,4-DBN	6574-99-8			127		1.37	1.6	7.4	**[2]**
3,4-DCT	95-75-0		>450	79/86		5.6			**[2]**
2,6-DFBN	1897-52-5			80					**[2]**
2,6-DFT	443-84-5			9/24		4.42			**[2]**
Toluene	108-88-3	10	535	4.			1.2	7	
Benzonitrile	100-47-0	1		72.					[6]
CO2	124-38-9		d.n.e.	d.n.e.			d.n.e.	d.n.e.	**[2]**
HCl	7647-01-0								**[2]**
HF	7664-39-3					0.836			**[2]** [4]
HBr	10035-10-6				90	3.345			**[2]**
HCN	74-90-8			-18					**[2]**
N2	7727-37-9		d.n.e.	d.n.e.		1.159	d.n.e.	d.n.e.	**[2]**
HCl (aq)	7647-01-0	210				1.553			**[2]**
HF(aq)	7664-39-3	14				2.21			**[2]**
HBr(aq)	10035-10-6					3.345			**[2]**

[1] At 101.3 kPa, 21°C, kg/m3
[2] MSDS/ICSC available
[3] relative density (air) = 0.6
[4] relative density (air) = 0.7
[5] Data from MSDS/ICSC unless mentioned
[6] Relative density (Air) =3.6

d.n.e. = does not exist (physically)
n.a. = not available

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Current Process

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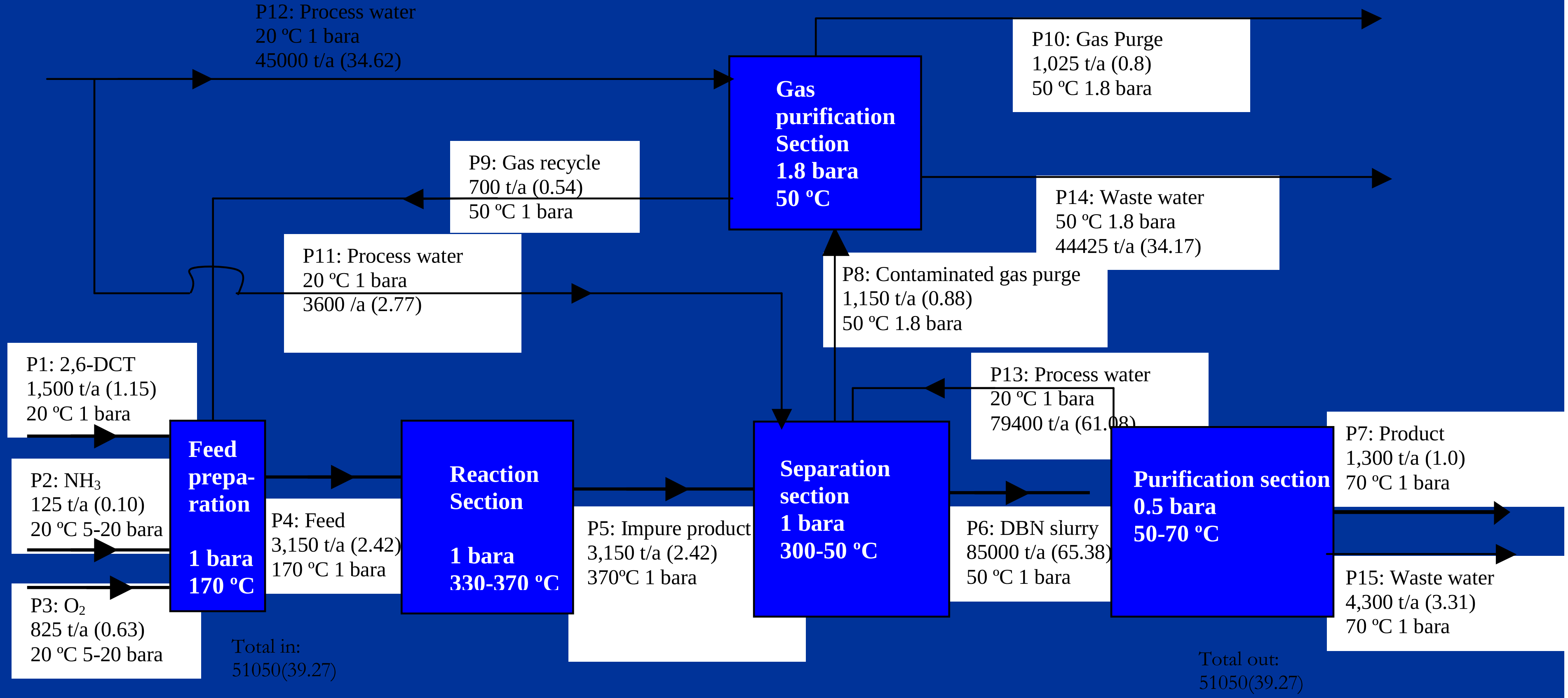

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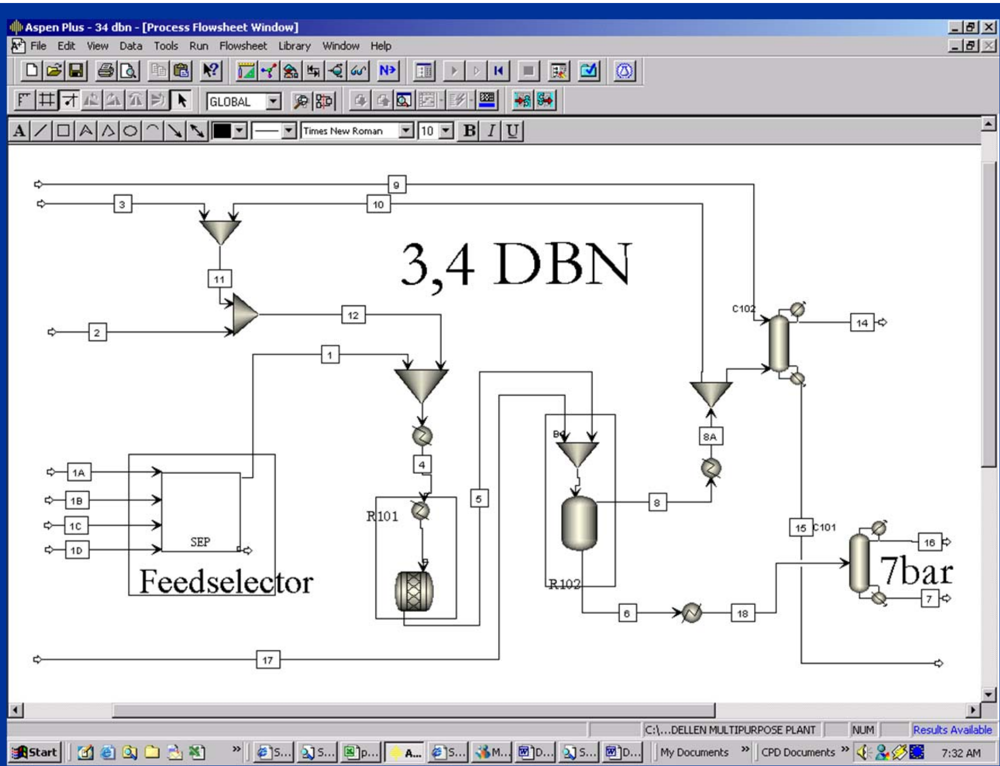
HF in equipment

- HF is no problem in diluted gas stream
  - HF content is no problem
  - (V = 0.004 & w, 0.00078% w)
  - 0.25 mm p/y corrosion, increase tube wall thickness a little

Aspen Model



Feedselector
The feedeslector is used to be able to switch feeds fast for modeling of the multipurpose plant
R101 Tube Reactor
The stoichometric reactor together with the heat exchanger model the Tube reactor cooled by the Salt melt.
C103 Quench
The Quench is modeled by an adiabetic mixer and a flash vessel with set in and outlet pressure.
C102 Gas Absorber
The gas absorber is modeled by a RADFRAC with one stream entering at the top and one at the bottom. No condensor or reboiler is used.
C101 Distillation Column
The distillation column is modeled with a RADFRAC
Quench Controller
The quench temperature is controlled by the nitrogen feed to the Quench. The set-point for the quench temperature is entered in a design spec that keeps the internal stream of the quench at set-point by varying the nitrogen feed.

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Block Scheme

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4 Coningen